1,3,5-Cycloheptatriene

544-25-2 | DTXSID5073909

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.54

Global applicability domain: Inside

Local applicability domain index: 6.96e-01

Confidence level: 6.72e-01

Nearest Neighbors from the Training Set

Image not found
1,3,5-Cycloheptatriene
Measured: 2.63
Predicted: 2.54

Image not found
1,3,5,7-Cyclooctatetraene
Measured: 3.08
Predicted: 2.81

Image not found
Styrene oxide
Measured: 1.61
Predicted: 2.11

Image not found
2,3-Dihydrobenzofuran
Measured: 2.14
Predicted: 2.10